Chemistry and Materials Science
Directorate News

Providing scientific excellence and leadership that meets and anticipates the needs of the Laboratory's programs

Summer 2004
Vol. 2, No. 3
Published quarterly

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Message from the Associate Director

For those of you who are involved in this year's LDRD competition, you may have seen marked changes in the proposal process. The most notable change this year was the addition of an open two-day LDRD Symposium in March, where we saw significantly increased participation from the broad CMS community. Other measures have also been put in place to improve communication and enhance the transparency of the process.

This month, the final exploratory-research (ER) proposals are being presented to the Lab-wide ER committee. We expect to receive comments from that committee on all of the CMS projects within the next few weeks.

Key criteria for evaluating and selecting LDRD projects continue to be the quality of the science and its alignment with both CMS and Lab-wide strategic plans, the quality of the teams executing the projects, and the

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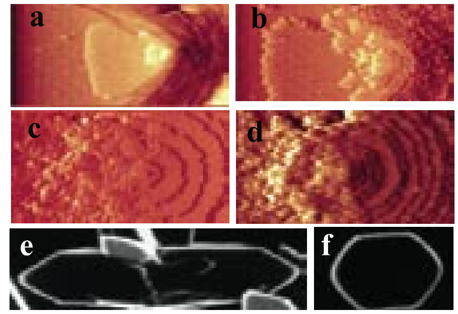
Corner on Science

An Up-Close Look at Kidney Stones

Kidney stones can be an excruciatingly painful affliction and are an all too common chronic disorder. Calcium oxalate monohydrate (COM), the primary component in most kidney stones, occurs in normal human urine, routinely creating tiny crystals. But several other molecules also naturally occur in urine to inhibit the development of the tiny crystals into larger kidney stones. Unfortunately, these inhibitors don't work for everyone.



Representative images showing the effect of citrate on COM morphology over time.

CMS postdoc **Roger Qiu** has been leading an investigation of how two molecules associated with kidney stones interact with crystals of COM. Qiu and colleagues **Chris Orme** and **Jim De Yoreo** used atomic force microscopy combined with molecular modeling to provide the first molecular-scale views of COM crystallization in the presence of citrate, a naturally occurring inhibitor that is also commonly prescribed to patients to reduce the growth of their stones, and osteopontin, a protein that is always found with stones but whose function is not well defined. The Livermore team is collaborating with several universities that have been examining the effects of these and other molecules on bulk samples of calcium oxalate monohydrate.

What Qiu discovered is that citrate and osteopontin work very differently on calcium oxalate crystals, each attacking a different face of the three-faced COM crystal. Citrate "docks" to the top of the crystal, where it drastically changes the crystal's shape (see figure above). A triangular, stepped hillock of crystal became quite

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Interview With...

Chris Orme

The latest news about **Chris Orme** is her recent 2002 Presidential Early Career Award for Scientists and Engineers (PECASE). Among 57 awardees from across the country, 7 were from the Department of Energy with 2 from Lawrence Livermore, Chris and **Edmond Chow** (Computations).

May 5 was the big day for Chris in Washington, D.C. In the morning, Energy Secretary Spencer Abraham honored the DOE awardees and their families at a special ceremony at DOE headquarters. The afternoon saw Chris and her mother (just one guest apiece) at the Old Executive Building where the President's Science Adviser, John H. Marburger III, recognized the awardees for the outstanding work they have achieved early in their careers and their potential for future leadership. Chris was honored "for her work in understanding the physical mechanisms of biomineralization and the development of force microscopy-based methods of investigating mineralization at the nanoscale."

The official White House award includes a plaque and—here's the best part—funding for a postdoc for five years. Chris is thrilled to have support for learning more about how biological materials develop.

Chris's own arrival at Livermore as a postdoc came about by accident. As a

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CHEMISTRY AND MATERIALS SCIENCE DIRECTORATE

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Lawrence Livermore National Laboratory
P.O. Box 808, L-090
Livermore, CA 94551
http://www-cms.llnl.gov/

UCRL-MI-205861-VOL-2-3

Publication Manager
Theresa Healy

Managing Editor
Katie Walter

Consulting Editor
Stephanie Shang

Scientific Editor
Michael Fluss

Contributing Editor
Emmeline Chen

Publication Design and Layout
Missy Davidson

Photographer
Marleen Emig

Graphics
Missy Davidson
Scott Dougherty
Marleen Emig

To be added to the internal distribution list for this newsletter, contact Stephanie Shang (ext. 3-0790 or shang2@llnl.gov).

A PDF of this newsletter with clickable Web links can be downloaded from the CMS Web site: http://www-cms.llnl.gov/news/newsletter.html.

This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

National Nuclear Security Administration

Notable Publications BY MICHAEL FLUSS

Interstellar Organic Matter

No, this is not about ET. It's about understanding the origin of organic compounds found in interplanetary dust particles (IDPs). Researchers from the Laboratory for Space Science, Washington University, St. Louis, and CMS and the Institute for Geophysics and Planetary Physics (IGPP) at LLNL used an armamentarium of advanced analytical tools (FIBs, NanoSIMS, TEMs, and the ALS) to determine the carbon and nitrogen isotopic composition and structural morphology of an IDP collected in Earth's atmosphere. They announced their findings in *Science* (**303**, 1355–1358 [2004]). CMS researcher **Zu Rong Dai** is a co-investigator with **John Bradley**, **Sasa Bajt**, and **Giles Graham** of IGPP.

By observing the presence of a ^{13}C depletion associated with a ^{15}N enrichment in an IDP named Benavente (yes, they name their dust particles), the authors are able to suggest that the anomalies are carried by heteroatomic organic compounds. Theoretical models indicate that low-temperature formation of organic compounds in cold interstellar molecular clouds can produce carbon and nitrogen fractionations. The authors note that more work will be required to confirm the generality of their model and whether the specific effects observed can be reproduced. The observation of a ^{13}C depletion associated with a ^{15}N enrichment in Benavente shows that C isotopic fractionation does occur and requires processes that can produce both effects in the same material, thus establishing an important constraint on the nature of interstellar chemistry.

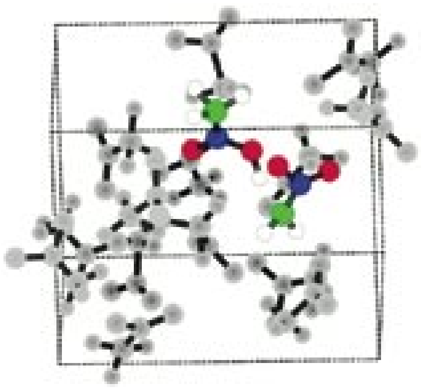
Zu Rong Dai

Publication URL:
http://www.sciencemag.org/cgi/reprint/303/5662/1355.pdf

Simulating HE Compost

Livermore scientists are ever on the look out for a better understanding of the decomposition mechanisms of high explosives. Recent work by CMS's **Riad Manaa** and **Larry Fried** with **Giulia Galli** of PAT, **Francois Gygi** of Computations, and **Even Reed** of the Massachusetts Institute of Technology reveals some of the early chemical activity of nitromethane (CH_3NO_2) under the very hot, dense conditions that accompany detonation. Their results were recently announced in the *Journal of Chemical Physics* (**120**, 10146–10153 [1 June 2004]).

The team's molecular dynamics simulations show that the first step in the decomposition process near the Chapman-Jouget state is not the breaking of the weak CN bond, which is typically the first bond to break in the gas phase. Instead, in this highly condensed phase, the strongest bond—CH—breaks. The nitromethane molecule is transformed into $CH_3NO_2H^+$, the aci ion $H_2CNO_2^-$, and the aci acid H_2CNO_2H, as shown in the figure. The simulations established these decomposition species for neat nitromethane for the first time.



A snapshot of the molecular dynamic simulation at 59 femtoseconds where the formation of $CH_3NO_2H^+$ and H_2CNO_2 takes place.

Publication URL:
http://scitation.aip.org/jcpo/?jsessionid=1309171091219926279 ■

Please send items for the Fall newsletter (e.g., directorate news, awards, conference calendar items) to **Stephanie Shang** (shang2@llnl.gov).

Directorate News

Summering at CMS

Spending lazy summer days at the beach is pure magic for some. But exploring pure and applied science with CMS mentors is the way our summer interns wanted to spend this summer. Seventy undergraduate and graduate students from all over the U.S. and several foreign countries have come to CMS through an array of programs: the Undergraduate Summer Institutes (USI), the Nuclear Science Internship Program (NSIP), the Computational Materials Science and Chemistry Summer Institute, and the more recently formed Energetic Materials Center (EMC). The various internship programs offer regular seminars that allow students to interact with distinguished scientists. Most programs have students work on a project and present their findings in a poster session at the end of the summer. Other students at CMS have been hired for the summer by individual scientist mentors to perform research.

To all of these students, we say WELCOME—and don't forget to take a little time off at the beach. ■

A few CMS summer students include (clockwise from top left) Bryan Bednarz (USI), Dan Spencer (USI), Paul Schuck (USI), Elaine Hart (EMC), and Diana Yi (USI). Laura Ludzigson (NSIP) is in the center.

Awards and Personnel News

Hello to New CMS Employees

From left, top row: MSTD physicist **Maximo Victoria**, MSTD postdoc **Trevor Willey**, CChED chemist **Greg Nyce**, MSTD postdoc **Sung Woo Yu**. Bottom row: CBN postdoc **Brian Dick**, CBN postdoc **Youngeun Kwon**, MSTD metallurgist **Janelle Gunther**, CBN administrative assistant **Josie Morgado**. Not pictured: CChED chemist **Yvon Araktingi**, and CChED postdoc **Thaddeus Norman**. ■

Saying Good-Bye to Our Retirees

CMS thanks the following individuals for their service to the Laboratory and wishes them a happy retirement!

Brynn Bollinger (CChED)
Sharon Crowder (CChED)
Dan McCright (MSTD) ■

DOE Award for Geoff Campbell and Vicki Mason-Reed

On June 8, **Geoff Campbell** and **Vicki Mason-Reed** received a 2002 Weapons Recognition of Excellence Award from the DOE's Dr. Everet Beckner, Deputy Administrator for Defense Programs.

Of 24 Laboratory employees receiving the award, just Geoff and Vicki were from CMS. The DOE presents the awards for outstanding contributions to the nation's nuclear weapons program.

Geoff and Vicki were members of the Case Dynamics Team, which developed two new experimental platforms and a suite of analysis tools and methodologies to study high-explosives-driven radiation-case dynamics.

Congratulations, Geoff and Vicki! ■

CMS metallurgist Geoff Campbell (back row, second from the right) and CMS senior technologist Vicki Mason-Reed (front row, third from the right) receive their DOE award.

CMS Graded “Outstanding” Yet Again BY JEFF KASS

The CMS Directorate Review Committee (DRC) has again given CMS “outstanding” grades for our scientific contributions. The May 5–7, 2004, review was chaired by Tom Tombrello of the California Institute of Technology, in his final act as DRC chairman. The DRC’s grade for CMS continues the high marks CMS has received over the past two years and is a tribute to the exceptional talent and hard work of our staff.

Introductory Session

Rokaya al Ayat, associate deputy director for science and technology, welcomed the committee and discussed the status of the Lab’s strategic planning process.

Tomás Díaz de la Rubia, CMS associate director, provided an update on our directorate since the last DRC meeting, focusing on the synergy among theory, experiment, and computations. Tomas distributed copies of the first phase of the CMS strategic plan and discussed how the themes addressed in the strategic plan mesh with Laboratory programs and research efforts.

High-Performance Scientific Computing

Chris Hollars (left) and DRC member Joanna Fowler of Brookhaven National Laboratory.

Presentations

Steve Ashby, deputy associate director for Computations, presented an overview of computational science at the Laboratory, including its integration into the Stockpile Stewardship Program and strengthening of the underlying science. The Thunder and the Blue Gene/L supercomputers will place the Laboratory at the forefront of computational science, allowing scientists to make breakthrough discoveries in many fields.

Wei Cai described how improvements in dislocation theories and the development of models are resulting in greatly improved predictions of materials behavior.

Chris Mundy discussed being able to simulate as many as 216 water molecules and, for the first time, obtain a stable liquid-vapor interface and a region of water below the interface.

Posters

Lawrence Fellow **Evan Reed** described the interaction of light with a shock wave in a photonic crystal. Predicted effects could lead to applications in optical communications, quantum computing, and shock diagnostics.

George Gilmer reviewed work that demonstrates how microstructural evolution in laser ablation is understood by atomic simulation. This pioneering simulation has broad implications for materials and nanostructure synthesis.

Jane Bearinger (right) with DRC chair Tom Tombrello of the California Institute of Technology.

Alexander Goncharov (left) and Nir Goldman.

Eduardo Bringa highlighted simulations and experiments that are clarifying dislocation mechanisms at extreme conditions.

Nir Goldman described water under extreme conditions of planetary interiors. Results offer a possible explanation for high magnetic fields observed in Neptune and Uranus.

Science in Support of Emerging Office of Science Programs in Genomes to Life and Biomolecular Materials

Presentations

Elbert Branscomb, associate director for Biology and Biotechnology Research Programs, described how microbial systems have been refined through competitive pressures to a point where certain essential features of the metabolic pathways must be shared. These shared features are of great interest for our biosecurity and environmental protection missions.

Jim De Yoreo described the BioSecurity and Nanotechnology Laboratory’s role in the Genomics:GTL (previously known as Genomes to Life) program. He highlighted current CMS efforts to partner with BBRP in initiatives aimed at insertion into Genomics:GTL.

Olgica Bakajin reported the first single-molecule, nonequilibrium observation of protein folding using detection of fluorescence resonance energy transfer. Folding was induced by abruptly changing from a denatured solution to a solution favoring the native folded state of the protein.

Julio Camarero discussed expressed protein ligation. His approach to protein immobilization offers the prospect of arraying proteins directly from cell lysates. The use of expressed protein ligation in isotopic labeling for nuclear magnetic resonance studies of complex protein structure was equally impressive.

Chris Orme highlighted her work with in situ atomic force microscopy to observe changes in crystal growth induced by impurity additions to the growth medium.

Posters

Alex Malkin and **Marco Plomb** described their efforts with atomic force microscopy to probe microorganisms under water and identify their spore species from surface architecture. Their new procedures for dissecting viruses to reveal internal structure have potential for identifying the origin of pathogens for attribution.

Alex Noy, **Todd Sulchek**, and **Tim Ratto** showed that interaction potentials can be extracted by measuring forces produced by pulling apart proteins and other complex molecules bound to the surface. Force spectroscopy provides a means for mapping the energy landscapes of complex molecules.

Alexander Malkin (left) and DRC member Rober Beaudet from the University of Southern California.

Chris Hollars described incorporating surface enhanced Raman spectra (SERS) nanosensors into prokariotic cells to measure various metabolic indicators. Chris's team demonstrated a nanoscale SERS-based pH measurement and showed that functionalized SERS particles can be localized within eukaryotic cells.

Jane Bearinger discussed use of surface modification techniques to control attachment of biological molecules. Selective attachment has been achieved by attaching specific peptides to the ends of PEG molecules using cross linkers.

New Elements Discovery

Ken Moody's overview of the history of elemental research covered everything from the early discoveries of elements 99 and 100 in thermonuclear bomb tests to the recent discovery of elements 113 and 115 with Russian scientists at the Dubna Laboratory as well as plans to explore even heavier elements.

Josh Patin described the synthesis of element 115. His discussion of the experiment conducted at Dubna to isolate and measure the atoms formed concluded with plans for future experiments. Work on element 115 was featured in the February 1, 2004, Sunday *New York Times*.

Strategy and Research Directions for Materials Science

Presentations

Christian Mailhiot described a vision for materials science research directions and an implementation roadmap of resource allocations centered on the dynamics of ultrafast materials processes, actinide science and strongly correlated materials, and nanoscale materials science and technology. The strategy is based on integrating experimental and high-performance computational efforts in support of current programs and anticipated future mission needs.

Joe Zaug (left) and DRC member Alexander King of Purdue University.

Kim Budil, currently in Washington, D.C., supporting the NNSA Office of Research, Development and Simulation, discussed DOE complex-wide directions for materials science, academic alliances in support of the ASCI program, and the NNSA university outreach program. Kim also indicated the scientific areas of opportunity for enhancing partnerships between Defense Programs and the Office of Science.

Jim Tobin discussed determining actinide electronic structures, emphasizing magnetic dipole behavior and the spin orbit splitting effect for plutonium. He showed that we are converging on the correct Hamiltonion for plutonium.

Tony van Buuren highlighted bucky diamonds, a new form of carbon. Tony provided a new understanding of the structure exhibited by nanoscale carbon clusters.

Jonathan Crowhurst discussed direct measurement of the speed of sound in iron under ultrahigh static pressure using a laser-induced ultrasonic wave technique coupled to a diamond anvil cell test. Wave propagation speeds were compared to seismic data from the Earth's core and mantle to show that propagation rates are consistent with cell results for pure iron.

John Elmer described subsecond, in situ observations of nonequilibrium phase formations at the atomic level during welding. He used spatially resolved x-ray diffraction to measure transient phase transformations that occur in the heated region around the weld pool.

Chris Orme and Jeff Tok.

Poster

Art Nelson highlighted the development and initial use of new capabilities for ultrafast measurement of materials properties.

External Collaborations and Participation

Dave Eaglesham gave the final talk, in which he described CMS strategic collaborations and broad participation in the scientific community. ■

Message from the Associate Director
Continued from page 1

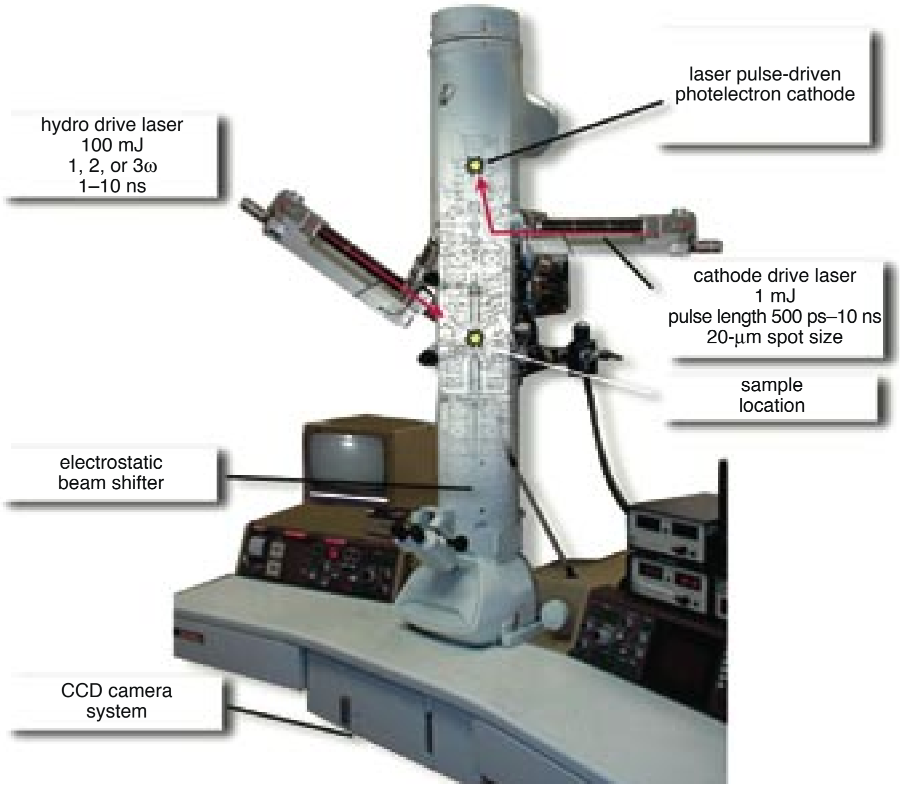
feasibility of each project's exit plan. In addition, we always encourage cross-directorate collaborations, and we have seen the overall funding of our LDRD projects increase significantly as a result over the last few years.

In the past year, we successfully funded projects that led to breakthroughs that will benefit both fundamental science and programs. Complete plutonium phonon dispersion data and computational advances with never-before-seen resolution are just two of the many groundbreaking discoveries that are dividends of our investments.

LDRD is an integral part of our overall investment portfolio. Acquisition of experimental equipment to meet the demands of current research is an equally important element. The new focused ion beam was installed in Building 235, and we expect this instrument to become a workhorse capability for new scientific and programmatic applications. We are striving to advance our leadership position in the investigation of ultrafast materials and chemical dynamics phenomena. Specifically, a new system incorporating both ultrafast electron diffraction and dynamic transmission electron microscopy is being developed and will be housed in Building 298.

The launch of the new Nanoscale Synthesis and Characterization Laboratory (NSCL) and its early accomplishments also resulted from our institutional investment strategy. The NSCL is a collaborative R&D environment and investment partnership between CMS and Engineering. The NSCL is initially focused on exploring the development of advanced materials and complex assemblies for future use in stewardship experiments and fusion ignition.

As the results of these investments come to fruition over the next few years, we look forward to further advancing the frontiers of sciences and meeting the evolving challenges of our national security mission. ■



The dynamic transmission electron microscope, an important element in the CMS investment strategy.

Postdoc News

Postdoc Symposium Results

The July 28 Postdoc Symposium was a great success! Thanks to everyone who spoke and presented posters.

During the symposium, **Joshua Patin** was honored with the third annual Hal Graboske Postdoctoral Award for the postdoc who has made the most outstanding contribution to our directorate and the Laboratory. The award for the best poster of the symposium went to **Nir Goldman**.

Contact **Tom Arsenlis** (ext. 4-2584), director of the CMS Postdoctoral Program, for more information.

Above: Postdoc Joshua Patin receives his award from Hal Graboske. Below: Postdoc Nir Goldman is presented with his award by Tom Arsenlis.

Postdoc People News

Let's welcome the following individuals who have become full-time Lab employees:

Kerri Blobaum (MSTD)
Tony Esposito (MSTD)
Brad Hart (CChED)

Adios to postdocs who have left the Lab:

Alex Ziegler (MSTD)
Stephen Glade (MSTD) ■

Laboratory Directed Research and Development at CMS

A contributor in LDRD: Jean Moran

The nuclear fission product ^{129}I is a long-lived radioactive contaminant that is biologically and chemically active in natural systems. ^{129}I is also a potential tracer of nuclear-fuel reprocessing activity, an application being explored by CMS scientist **Jean Moran** in her LDRD project, “Transport and biogeochemical cycling of iodine-129 from nuclear fuel reprocessing facilities.” This Exploratory Research in the Directorates project, which is sponsored by CMS, is being conducted in association with researchers from the Energy & Environment Directorate at the Laboratory’s Center for Accelerator Mass Spectrometry.

Together with her team of scientists from CBN—**Max Hu**, **Erick Ramon**, **Ross Williams**, and **Pihong Zhao**—and **Erik Nelson** from MSTD, Jean is investigating where ^{129}I tends to reside on Earth and how the radionuclide is transported and cycled through the global environment. This information can then be used to interpret the various concentrations of ^{129}I found throughout the world. Such analyses could provide valuable details about who in our global community is reprocessing nuclear fuel, how much fuel is being reprocessed, and where this activity is occurring.

The team’s LDRD results can also be applied to environmental studies of ^{129}I contamination at Department of Energy legacy sites, such as the Nevada Test Site. Understanding the transport and cycling mechanisms of ^{129}I will assist researchers in conducting long-term dose assessments to determine the future effects of radionuclide contamination. Information about ^{129}I is also relevant to feasibility studies of Yucca Mountain as a nuclear repository.

After graduating in 1986 from the University of Washington, Seattle, with a master’s degree in geophysics, Jean joined the U.S. Peace Corps and lived in Fiji for four years. She taught high school physics and math courses and trained Peace Corps volunteers. Jean then returned to her undergraduate alma mater, the University of Rochester and began pursuing her Ph.D. in geochemistry.

Jean’s dissertation involved using accelerator mass spectrometry to measure ^{129}I. She continued to investigate ^{129}I as part of her postdoctoral work on the global cycling of radionuclides at Texas A&M University and then joined CMS in 1997. Her background fit perfectly with CMS’s need for a specialist in isotope hydrology. Jean’s previous studies have used radioactive isotopes to examine groundwater flow and water quality. She looks forward to exploring a wider range of tracers and to discovering what happens downstream or downwind of a nuclear release point. ■

Interview With...
Continued from page 1

physics graduate student at the University of Michigan, she primarily studied crystal growth in ultrahigh vacuum environments. She had also begun simulating the protein folding process and hoped to work with biological systems. CMS’s **Jim De Yoreo** asked her advisor to give a talk at Livermore. He couldn’t make it and sent Chris in his stead. De Yoreo had work for a postdoc in biological mineral growth, Chris’s visit turned into an interview, and the next thing Chris knew, she was a postdoc at Livermore.

Today Chris is scientific capability leader for the Biophysical and Interfacial Sciences Group. Her postdoc work with calcium carbonate segued into examining metals for hip and dental implants and eventually to work with the same metals but this time for waste canisters at Yucca Mountain. Chris notes that the interior of the human body and the environment inside Yucca Mountain are remarkably similar. Both are quite salty, for example. Human cells produce hydrogen peroxide when they are inflamed, as they would be with a new implant. Hydrogen peroxide is likewise a product of radiation passing through water and will be part of any corrosion that appears on Yucca Mountain waste canisters. Chris is one of the lead scientists for corrosion studies for the Yucca Mountain project.

With external funding from the National Institutes of Health, Chris is also researching the growth of biological minerals. She is currently studying calcium phosphate, of which bones and teeth are made, and calcium oxalate, the primary constituent of kidney stones. Chris and her team members use atomic force microscopy to make movies of crystal growth in real time as solution flows over the crystal. Precise environmental conditions are essential for this painstaking process to work.

Soon Chris will reap what she has sown with her hard work to date on biomineralization. Together with a newly hired postdoc, funded through the PECASE award by the DOE and its Office of Basic Energy Science, she will continue the research she loves and, she hopes, make an important discovery or two. ■

Conference Calendar

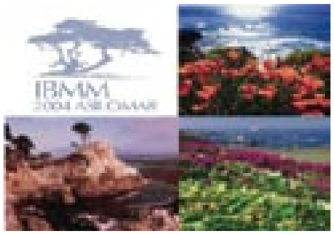
DATE	CONFERENCE	LOCATION	WEB SITE
September 5–10, 2004	Fourteenth International Conference on Ion Beam Modification of Materials	Monterey, CA	http://chapters.avs.org/nccavs/ibbm
October 11–15, 2004	2nd International Conference on Multiscale Materials Modeling	Los Angeles, CA	http://osiris.seas.ucla.edu/mmm/

Fourteenth International Conference on Ion Beam Modification of Materials

The IBMM conference, co-sponsored this year by LLNL, is the major international forum to present and discuss recent research results and future directions in the field of ion-beam modification, synthesis, and characterization of materials.

Topics will include:

- Fundamentals of ion-solid interactions, modeling, simulation, and theory
- Ion beam processing of semiconductors, metals, ceramics, and polymers
- Application of ion beams to electronic, magnetic, and optical materials and devices
- Processing and synthesis with cluster ion beams
- Plasma-immersion ion implantation for surface modification and surface coating
- Novel ion beam processing and applications
- Manipulation and control of materials at the nanometer scale, and synthesis and modifications of biomaterials and other novel materials.



The CMS Directorate is playing a major role in the organization of the event, which will be held in picturesque Monterey. **Tomás Díaz de la Rubia**, AD for CMS, and **Alex Hamza**, director of the Nanoscale Synthesis and Characterization Laboratory, are two of four co-chairs on the Organizing Committee. **Tom Felter**, **Dave Eaglesham**, and **Sergei Kucheyev** in CMS and **Graham Bench**, from Energy & Environment, are coordinating many of the local arrangements. ■

Corner on Science
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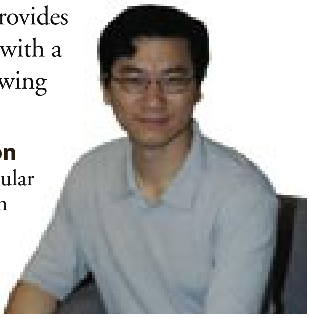
rounded and disc shaped. But citrate had less effect on the other two sides of the COM crystal. These data along with theoretical calculations suggest that citrate modifies the shape and inhibits the growth of COM as a direct result of pinning step motion on the top face.

Osteopontin, in contrast, had the most effect on the side face of the COM crystal but had little effect on the top face where citrate had been so helpful. Osteopontin also changed the shape and inhibited the growth of the side face of the COM crystal.

Qiu is excited about the results of this research for both the medical community and materials science. For the creation of new drugs to treat kidney stones, a combination of citrate and osteopontin, which affect different faces of COM, may prove to have an additive effect to stop the growth of stones. The knowledge that these modifiers are so effective at changing the shape of a crystal provides materials scientists with a mechanism for growing "designer" crystals.

Related Publication

Qiu, S.R. et al. Molecular modulation of calcium oxalate crystallization by ostopontin and citrate. *PNAS* **101** 7, 1811-1815 (2004). (**Cover article**). ■


CMS postdoc Roger Qiu.

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